

Fumaric acid, 2-phenethyl 8-chlorooctyl ester

Inchi: InChI=1S/C20H27ClO4/c21-15-8-3-1-2-4-9-16-24-19(22)12-13-20(23)25-17-14-18-10-6-5
InchiKey: CJCFTGRBPEAMS-OUKQBFOZSA-N
Formula: C20H27ClO4
SMILES: O=C(C=CC(=O)OCCc1ccccc1)OCCCCCCCCCl
Mol. weight [g/mol]: 366.88

Physical Properties

Property code	Value	Unit	Source
gf	-169.62	kJ/mol	Joback Method
hf	-607.72	kJ/mol	Joback Method
hfus	51.57	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.451		Crippen Method
mvol	291.720	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	2802.00		NIST Webbook
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tb	877.85	K	Joback Method
tc	1086.06	K	Joback Method
tf	510.74	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.55	J/molxK	877.85	Joback Method
cpg	893.16	J/molxK	912.55	Joback Method
cpg	906.71	J/molxK	947.25	Joback Method
cpg	919.23	J/molxK	981.96	Joback Method
cpg	930.77	J/molxK	1016.66	Joback Method
cpg	941.38	J/molxK	1051.36	Joback Method
cpg	951.09	J/molxK	1086.06	Joback Method
dvisc	0.0005191	Paxs	510.74	Joback Method

dvisc	0.0002705	Paxs	571.92	Joback Method
dvisc	0.0001599	Paxs	633.11	Joback Method
dvisc	0.0001037	Paxs	694.29	Joback Method
dvisc	0.0000721	Paxs	755.48	Joback Method
dvisc	0.0000530	Paxs	816.66	Joback Method
dvisc	0.0000406	Paxs	877.85	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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